



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2024 – 10:14 AM EDT

PDB ID : 8VS8  
Title : Crystal structure of ADI-19425 Fab in complex with anti-idiotypic 1D3 Fab  
Authors : Kher, G.; Homad, L.J.; McGuire, A.T.; Pancera, M.  
Deposited on : 2024-01-23  
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

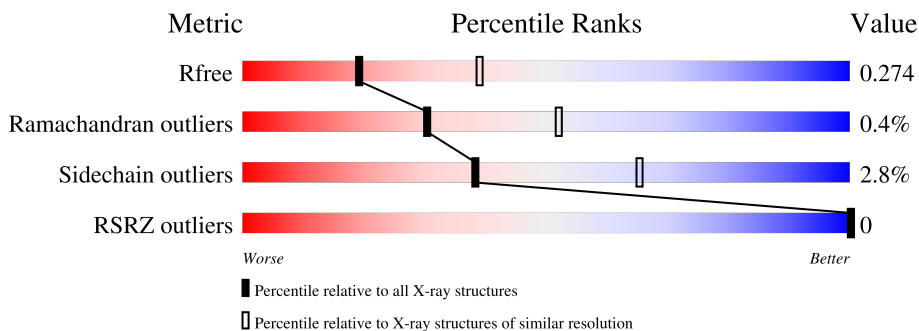
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





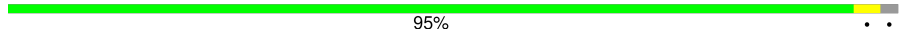
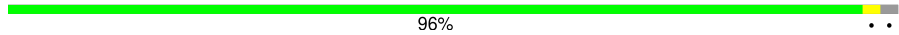

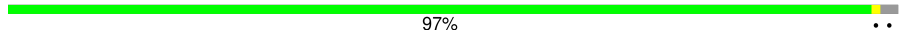




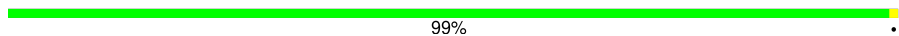
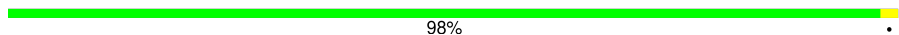
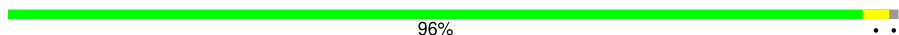
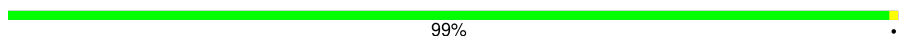


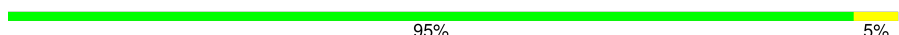
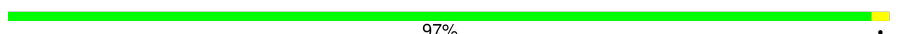
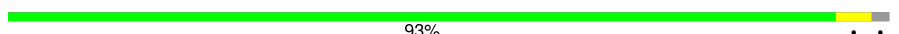
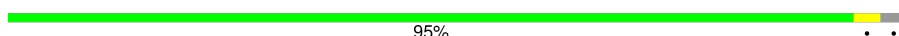
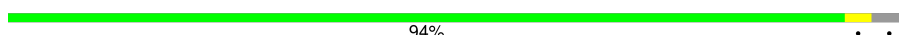




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	4708 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	
1	E	227	
1	I	227	
1	M	227	
1	Q	227	
1	U	227	

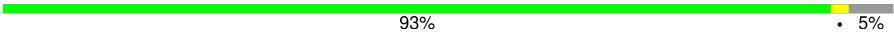
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Mol	Chain	Length	Quality of chain
1	Y	227	
1	c	227	
2	B	218	
2	F	218	
2	J	218	
2	N	218	
2	R	218	
2	V	218	
2	Z	218	
2	d	218	
3	C	214	
3	G	214	
3	K	214	
3	O	214	
3	S	214	
3	W	214	
3	a	214	
3	e	214	
4	D	226	
4	H	226	
4	L	226	
4	P	226	
4	T	226	
4	X	226	
4	b	226	

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Mol	Chain	Length	Quality of chain
4	f	226	 93% • 5%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 45030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ADI-19425 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	Total 1512	C 958	N 253	O 293	S 8	0	0	0
1	E	206	Total 1547	C 979	N 259	O 301	S 8	0	0	0
1	I	121	Total 920	C 578	N 156	O 180	S 6	0	0	0
1	M	210	Total 1576	C 996	N 264	O 308	S 8	0	0	0
1	Q	125	Total 940	C 588	N 159	O 187	S 6	0	0	0
1	U	178	Total 1347	C 850	N 227	O 262	S 8	0	0	0
1	Y	121	Total 920	C 578	N 156	O 180	S 6	0	0	0
1	c	98	Total 748	C 474	N 126	O 143	S 5	0	0	0

- Molecule 2 is a protein called ADI-19425 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total 1568	C 983	N 261	O 320	S 4	1	0	0
2	F	214	Total 1587	C 996	N 263	O 324	S 4	1	0	0
2	J	110	Total 802	C 502	N 133	O 165	S 2	0	0	0
2	N	214	Total 1581	C 993	N 260	O 324	S 4	1	0	0
2	R	110	Total 806	C 504	N 134	O 166	S 2	0	0	0
2	V	201	Total 1484	C 933	N 245	O 302	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	108	Total	C	N	O	S	0	0	0
			792	496	131	163	2			
2	d	81	Total	C	N	O	S	0	0	0
			602	379	97	124	2			

- Molecule 3 is a protein called 1D3 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1649	1027	279	338	5			
3	G	214	Total	C	N	O	S	0	0	0
			1649	1027	280	337	5			
3	K	212	Total	C	N	O	S	0	0	0
			1641	1024	279	334	4			
3	O	214	Total	C	N	O	S	0	0	0
			1657	1032	281	339	5			
3	S	214	Total	C	N	O	S	0	0	0
			1647	1026	277	339	5			
3	W	200	Total	C	N	O	S	0	0	0
			1549	967	261	317	4			
3	a	214	Total	C	N	O	S	0	0	0
			1645	1023	278	339	5			
3	e	214	Total	C	N	O	S	0	0	0
			1635	1018	275	337	5			

- Molecule 4 is a protein called 1D3 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	221	Total	C	N	O	S	9	0	0
			1660	1053	274	327	6			
4	H	220	Total	C	N	O	S	0	0	0
			1648	1047	270	325	6			
4	L	218	Total	C	N	O	S	2	0	0
			1632	1036	271	319	6			
4	P	217	Total	C	N	O	S	3	0	0
			1637	1041	270	320	6			
4	T	214	Total	C	N	O	S	2	0	0
			1616	1029	266	315	6			
4	X	216	Total	C	N	O	S	0	0	0
			1622	1031	266	319	6			
4	b	218	Total	C	N	O	S	5	0	0
			1639	1041	270	322	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	f	215	1594	1014	260	314	6	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total 9	O 9	0	0
5	B	7	Total 7	O 7	0	0
5	C	5	Total 5	O 5	0	0
5	D	13	Total 13	O 13	0	0
5	E	6	Total 6	O 6	0	0
5	F	6	Total 6	O 6	0	0
5	G	10	Total 10	O 10	0	0
5	H	6	Total 6	O 6	0	0
5	I	5	Total 5	O 5	0	0
5	J	1	Total 1	O 1	0	0
5	K	3	Total 3	O 3	0	0
5	L	6	Total 6	O 6	0	0
5	M	14	Total 14	O 14	0	0
5	N	5	Total 5	O 5	0	0
5	O	13	Total 13	O 13	0	0
5	P	2	Total 2	O 2	0	0
5	Q	6	Total 6	O 6	0	0
5	S	5	Total 5	O 5	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	T	8	Total O 8 8	0	0
5	U	5	Total O 5 5	0	0
5	V	4	Total O 4 4	0	0
5	W	7	Total O 7 7	0	0
5	X	6	Total O 6 6	0	0
5	Y	3	Total O 3 3	0	0
5	Z	1	Total O 1 1	0	0
5	a	7	Total O 7 7	0	0
5	b	10	Total O 10 10	0	0
5	c	2	Total O 2 2	0	0
5	e	2	Total O 2 2	0	0
5	f	1	Total O 1 1	0	0

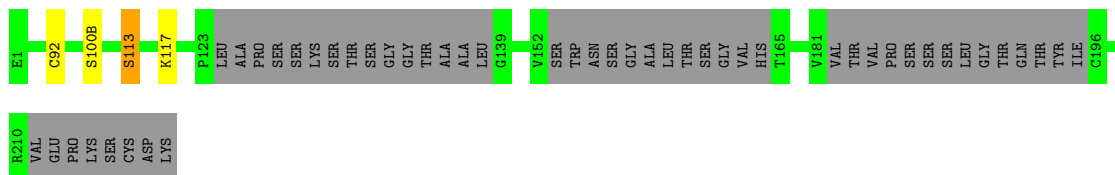





SER GLY VAL HIS THR PHE PRO PRO VAL VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR THR VAL VAL THR THR VAL PRO SER SER SER LEU THR GLN THR TYR ILE ILE ASN ASN VAL ASN HIS LYS PRO PRO SER SER ASN THR THR LYS VAL ASP LYS ARG VAL GLU PRO LYS SER CYS ASP LYS

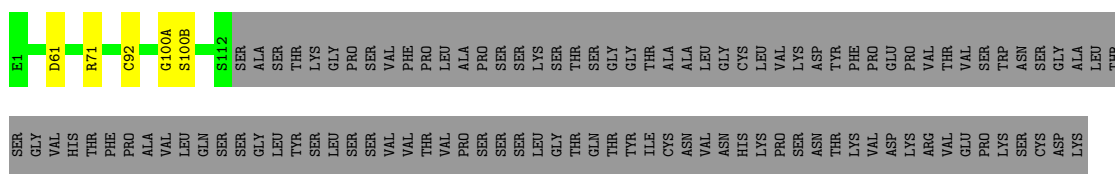
- Molecule 1: ADI-19425 Heavy Chain

Chain U:  77% 22%



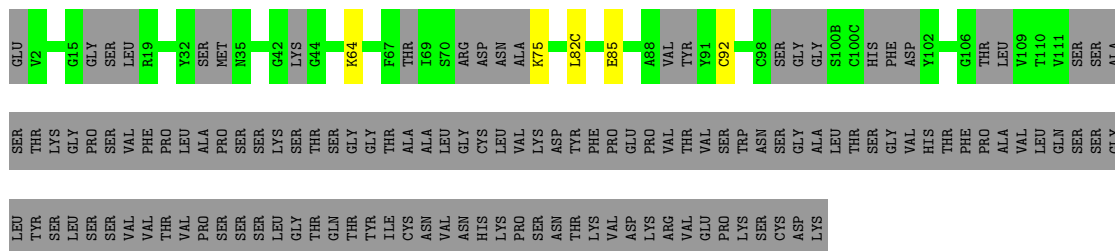
- Molecule 1: ADI-19425 Heavy Chain

Chain Y:  51% 47%



- Molecule 1: ADI-19425 Heavy Chain

Chain c:  41% 57%



- Molecule 2: ADI-19425 Light Chain

Chain B:  95%



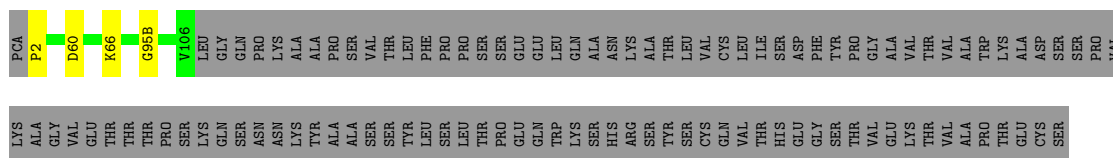
- Molecule 2: ADI-19425 Light Chain

Chain F:  96%



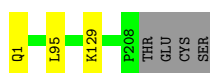
- Molecule 2: ADI-19425 Light Chain

Chain J:  49% 50%



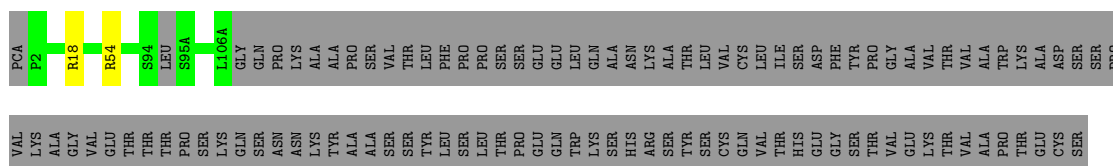
- Molecule 2: ADI-19425 Light Chain

Chain N:  97%




- Molecule 2: ADI-19425 Light Chain

Chain R:  50% 50%



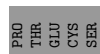
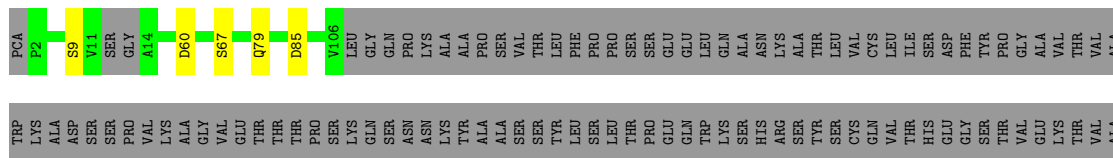
- Molecule 2: ADI-19425 Light Chain

Chain V:  90% 8%



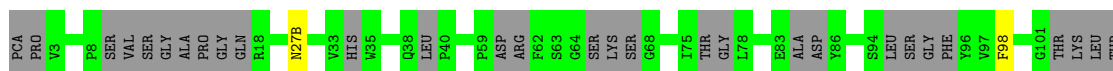
- Molecule 2: ADI-19425 Light Chain

Chain Z:  47% 50%

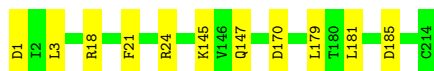


- Molecule 2: ADI-19425 Light Chain

Chain d:  36% 63%







- Molecule 3: 1D3 Light Chain



- Molecule 4: 1D3 Heavy Chain



- Molecule 4: 1D3 Heavy Chain



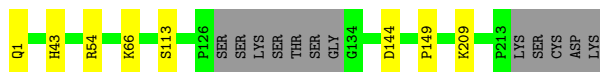
- Molecule 4: 1D3 Heavy Chain



- Molecule 4: 1D3 Heavy Chain

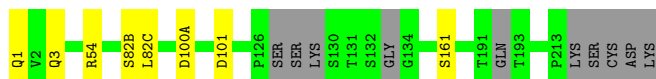


- Molecule 4: 1D3 Heavy Chain



- Molecule 4: 1D3 Heavy Chain





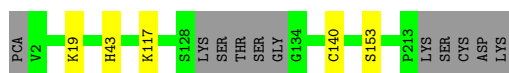
- Molecule 4: 1D3 Heavy Chain

Chain b: 95%



- Molecule 4: 1D3 Heavy Chain

Chain f: 93% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.07Å 149.98Å 164.43Å 83.98° 89.90° 74.61°	Depositor
Resolution (Å)	49.33 – 2.67 49.33 – 2.67	Depositor EDS
% Data completeness (in resolution range)	92.5 (49.33-2.67) 92.5 (49.33-2.67)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.231 , 0.273 0.232 , 0.274	Depositor DCC
$R_{free}$ test set	11499 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtrriage
Anisotropy	0.250	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	45030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
PCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/1548	0.50	0/2105
1	E	0.30	0/1584	0.51	0/2153
1	I	0.26	0/941	0.50	0/1272
1	M	0.26	0/1614	0.50	0/2195
1	Q	0.26	0/961	0.52	0/1301
1	U	0.29	0/1377	0.56	1/1863 (0.1%)
1	Y	0.25	0/941	0.50	0/1272
1	c	0.27	0/757	0.48	0/1010
2	B	0.26	0/1609	0.49	0/2201
2	F	0.26	0/1621	0.48	0/2218
2	J	0.25	0/822	0.48	0/1121
2	N	0.26	0/1615	0.49	0/2211
2	R	0.25	0/825	0.47	0/1123
2	V	0.27	0/1512	0.48	0/2064
2	Z	0.26	0/811	0.48	0/1106
2	d	0.26	0/610	0.49	0/820
3	C	0.26	0/1685	0.51	0/2288
3	G	0.25	0/1685	0.50	0/2288
3	K	0.25	0/1677	0.49	0/2277
3	O	0.25	0/1693	0.50	0/2297
3	S	0.26	0/1683	0.50	0/2286
3	W	0.25	0/1582	0.51	0/2145
3	a	0.27	0/1681	0.53	0/2285
3	e	0.26	0/1671	0.50	0/2273
4	D	0.29	0/1697	0.51	0/2314
4	H	0.26	0/1684	0.49	0/2296
4	L	0.27	0/1667	0.49	0/2272
4	P	0.28	0/1673	0.51	0/2280
4	T	0.28	0/1652	0.53	0/2253
4	X	0.26	0/1656	0.49	0/2257
4	b	0.27	0/1675	0.51	0/2284
4	f	0.27	0/1637	0.52	0/2237



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.27	0/45846	0.50	1/62367 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	113	SER	N-CA-CB	5.17	118.26	110.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/227 (87%)	183 (93%)	12 (6%)	2 (1%)	13	29
1	E	200/227 (88%)	193 (96%)	6 (3%)	1 (0%)	25	46
1	I	119/227 (52%)	114 (96%)	4 (3%)	1 (1%)	16	35
1	M	204/227 (90%)	197 (97%)	6 (3%)	1 (0%)	25	46
1	Q	123/227 (54%)	119 (97%)	2 (2%)	2 (2%)	8	18
1	U	170/227 (75%)	155 (91%)	13 (8%)	2 (1%)	11	25
1	Y	119/227 (52%)	113 (95%)	4 (3%)	2 (2%)	7	17
1	c	78/227 (34%)	72 (92%)	6 (8%)	0	100	100
2	B	211/218 (97%)	197 (93%)	14 (7%)	0	100	100
2	F	212/218 (97%)	200 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	108/218 (50%)	99 (92%)	8 (7%)	1 (1%)	14	32
2	N	212/218 (97%)	198 (93%)	14 (7%)	0	100	100
2	R	106/218 (49%)	96 (91%)	10 (9%)	0	100	100
2	V	191/218 (88%)	176 (92%)	14 (7%)	1 (0%)	25	46
2	Z	104/218 (48%)	96 (92%)	8 (8%)	0	100	100
2	d	63/218 (29%)	55 (87%)	8 (13%)	0	100	100
3	C	212/214 (99%)	201 (95%)	11 (5%)	0	100	100
3	G	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	K	210/214 (98%)	199 (95%)	10 (5%)	1 (0%)	25	46
3	O	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	S	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
3	W	194/214 (91%)	178 (92%)	15 (8%)	1 (0%)	25	46
3	a	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
3	e	212/214 (99%)	198 (93%)	13 (6%)	1 (0%)	25	46
4	D	219/226 (97%)	210 (96%)	8 (4%)	1 (0%)	25	46
4	H	216/226 (96%)	205 (95%)	11 (5%)	0	100	100
4	L	214/226 (95%)	205 (96%)	8 (4%)	1 (0%)	25	46
4	P	213/226 (94%)	203 (95%)	10 (5%)	0	100	100
4	T	210/226 (93%)	197 (94%)	12 (6%)	1 (0%)	25	46
4	X	208/226 (92%)	198 (95%)	8 (4%)	2 (1%)	13	29
4	b	214/226 (95%)	200 (94%)	14 (6%)	0	100	100
4	f	211/226 (93%)	200 (95%)	11 (5%)	0	100	100
All	All	5798/7080 (82%)	5460 (94%)	317 (6%)	21 (0%)	30	52

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	100(A)	GLY
1	Q	115	SER
1	U	113	SER
1	A	100(B)	SER
1	A	114	ALA
1	E	100(B)	SER
4	L	101	ASP

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Mol	Chain	Res	Type
1	Q	100(B)	SER
1	U	100(B)	SER
2	V	199	GLY
1	Y	100(B)	SER
4	D	82(B)	SER
1	I	100(B)	SER
1	M	100(B)	SER
4	X	82(C)	LEU
3	K	76	ASN
3	W	80	SER
4	X	82(B)	SER
2	J	95(B)	GLY
3	e	52	SER
4	T	149	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	167/191 (87%)	163 (98%)	4 (2%)	44 70
1	E	173/191 (91%)	167 (96%)	6 (4%)	31 57
1	I	99/191 (52%)	99 (100%)	0	100 100
1	M	177/191 (93%)	174 (98%)	3 (2%)	56 79
1	Q	101/191 (53%)	96 (95%)	5 (5%)	20 42
1	U	151/191 (79%)	149 (99%)	2 (1%)	65 84
1	Y	99/191 (52%)	96 (97%)	3 (3%)	36 63
1	c	80/191 (42%)	75 (94%)	5 (6%)	15 32
2	B	174/181 (96%)	168 (97%)	6 (3%)	32 58
2	F	177/181 (98%)	174 (98%)	3 (2%)	56 79
2	J	88/181 (49%)	85 (97%)	3 (3%)	32 58
2	N	176/181 (97%)	174 (99%)	2 (1%)	70 86
2	R	89/181 (49%)	88 (99%)	1 (1%)	70 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	165/181 (91%)	163 (99%)	2 (1%)	67	85
2	Z	87/181 (48%)	82 (94%)	5 (6%)	17	37
2	d	66/181 (36%)	64 (97%)	2 (3%)	36	63
3	C	189/191 (99%)	186 (98%)	3 (2%)	58	80
3	G	189/191 (99%)	185 (98%)	4 (2%)	48	74
3	K	189/191 (99%)	184 (97%)	5 (3%)	41	68
3	O	191/191 (100%)	188 (98%)	3 (2%)	58	80
3	S	189/191 (99%)	186 (98%)	3 (2%)	58	80
3	W	180/191 (94%)	171 (95%)	9 (5%)	20	42
3	a	188/191 (98%)	177 (94%)	11 (6%)	16	35
3	e	186/191 (97%)	181 (97%)	5 (3%)	40	67
4	D	181/186 (97%)	173 (96%)	8 (4%)	24	48
4	H	179/186 (96%)	174 (97%)	5 (3%)	38	65
4	L	177/186 (95%)	173 (98%)	4 (2%)	45	72
4	P	178/186 (96%)	169 (95%)	9 (5%)	20	42
4	T	175/186 (94%)	169 (97%)	6 (3%)	32	58
4	X	176/186 (95%)	171 (97%)	5 (3%)	38	65
4	b	178/186 (96%)	176 (99%)	2 (1%)	70	86
4	f	171/186 (92%)	166 (97%)	5 (3%)	37	64
All	All	4985/5992 (83%)	4846 (97%)	139 (3%)	38	65

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	LYS
1	A	117	LYS
1	A	146	PHE
2	B	61	ARG
2	B	66	LYS
2	B	156	LYS
2	B	160	GLU
2	B	166	LYS
2	B	200	SER
3	C	7	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	22	SER
3	C	56	SER
4	D	13	ARG
4	D	17	SER
4	D	43	HIS
4	D	64	LYS
4	D	161	SER
4	D	197	ASN
4	D	199	ASN
4	D	201	LYS
1	E	92	CYS
1	E	115	SER
1	E	116	THR
1	E	140	CYS
1	E	197	ASN
1	E	209	LYS
2	F	15	PRO
2	F	166	LYS
2	F	180	LEU
3	G	21	PHE
3	G	24	ARG
3	G	61	ARG
3	G	122	ASP
4	H	66	LYS
4	H	81	GLN
4	H	192	GLN
4	H	197	ASN
4	H	201	LYS
2	J	2	PRO
2	J	60	ASP
2	J	66	LYS
3	K	21	PHE
3	K	67	SER
3	K	107	LYS
3	K	147	GLN
3	K	185	ASP
4	L	21	SER
4	L	61	GLU
4	L	94	ARG
4	L	206	LYS
1	M	19	ARG
1	M	197	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	210	ARG
2	N	95	LEU
2	N	129	LYS
3	O	45	ARG
3	O	61	ARG
3	O	105	GLU
4	P	23	LYS
4	P	43	HIS
4	P	54	ARG
4	P	81	GLN
4	P	129	LYS
4	P	161	SER
4	P	199	ASN
4	P	206	LYS
4	P	212	GLU
1	Q	25	SER
1	Q	46	GLU
1	Q	83	ARG
1	Q	92	CYS
1	Q	112	SER
2	R	18	ARG
3	S	1	ASP
3	S	21	PHE
3	S	45	ARG
4	T	43	HIS
4	T	54	ARG
4	T	66	LYS
4	T	113	SER
4	T	144	ASP
4	T	209	LYS
1	U	92	CYS
1	U	117	LYS
2	V	3	VAL
2	V	56	SER
3	W	18	ARG
3	W	21	PHE
3	W	45	ARG
3	W	54	SER
3	W	61	ARG
3	W	77	SER
3	W	107	LYS
3	W	108	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	W	142	ARG
4	X	3	GLN
4	X	54	ARG
4	X	100(A)	ASP
4	X	101	ASP
4	X	161	SER
1	Y	61	ASP
1	Y	71	ARG
1	Y	92	CYS
2	Z	9	SER
2	Z	60	ASP
2	Z	67	SER
2	Z	79	GLN
2	Z	85	ASP
3	a	1	ASP
3	a	3	LEU
3	a	18	ARG
3	a	21	PHE
3	a	24	ARG
3	a	145	LYS
3	a	147	GLN
3	a	170	ASP
3	a	179	LEU
3	a	181	LEU
3	a	185	ASP
4	b	51	ILE
4	b	66	LYS
1	c	64	LYS
1	c	75	LYS
1	c	82(C)	LEU
1	c	85	GLU
1	c	92	CYS
2	d	27(B)	ASN
2	d	98	PHE
3	e	3	LEU
3	e	18	ARG
3	e	52	SER
3	e	61	ARG
3	e	185	ASP
4	f	19	LYS
4	f	43	HIS
4	f	117	LYS

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Mol	Chain	Res	Type
4	f	140	CYS
4	f	153	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
2	B	108	GLN
1	E	197	ASN
2	F	79	GLN
2	J	79	GLN
2	N	108	GLN
1	Q	3	GLN
2	V	79	GLN
2	V	169	ASN
3	W	198	HIS
4	X	6	GLN
3	a	137	ASN
2	d	38	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PCA	H	1	4	7,8,9	0.59	0	9,10,12	1.02	1 (11%)
4	PCA	T	1	4	7,8,9	0.51	0	9,10,12	0.98	1 (11%)
2	PCA	V	1	2	7,8,9	0.46	0	9,10,12	1.27	1 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PCA	X	1	4	7,8,9	0.61	0	9,10,12	0.82	1 (11%)
4	PCA	P	1	4	7,8,9	0.52	0	9,10,12	0.91	1 (11%)
4	PCA	L	1	4	7,8,9	0.45	0	9,10,12	0.79	1 (11%)
4	PCA	b	1	4	7,8,9	0.60	0	9,10,12	1.19	1 (11%)
4	PCA	D	1	4	7,8,9	0.55	0	9,10,12	0.87	1 (11%)
2	PCA	N	1	2	7,8,9	0.48	0	9,10,12	1.24	1 (11%)
2	PCA	F	1	2	7,8,9	0.47	0	9,10,12	0.88	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCA	H	1	4	-	0/0/11/13	0/1/1/1
4	PCA	T	1	4	-	0/0/11/13	0/1/1/1
2	PCA	V	1	2	-	0/0/11/13	0/1/1/1
4	PCA	X	1	4	-	0/0/11/13	0/1/1/1
4	PCA	P	1	4	-	0/0/11/13	0/1/1/1
4	PCA	L	1	4	-	0/0/11/13	0/1/1/1
4	PCA	b	1	4	-	0/0/11/13	0/1/1/1
4	PCA	D	1	4	-	0/0/11/13	0/1/1/1
2	PCA	N	1	2	-	0/0/11/13	0/1/1/1
2	PCA	F	1	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	1	PCA	O-C-CA	-3.70	115.26	124.77
2	N	1	PCA	O-C-CA	-3.28	116.33	124.77
4	b	1	PCA	O-C-CA	-3.20	116.53	124.77
4	T	1	PCA	O-C-CA	-2.86	117.41	124.77
4	H	1	PCA	O-C-CA	-2.44	118.49	124.77
4	P	1	PCA	O-C-CA	-2.43	118.53	124.77
4	D	1	PCA	O-C-CA	-2.37	118.67	124.77
2	F	1	PCA	O-C-CA	-2.34	118.75	124.77
4	X	1	PCA	O-C-CA	-2.17	119.18	124.77
4	L	1	PCA	O-C-CA	-2.17	119.19	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	203/227 (89%)	-1.63	0 100 100	24, 40, 88, 103	0
1	E	206/227 (90%)	-1.64	0 100 100	24, 41, 75, 88	0
1	I	121/227 (53%)	-1.64	0 100 100	29, 45, 63, 83	0
1	M	210/227 (92%)	-1.63	0 100 100	26, 43, 73, 87	0
1	Q	125/227 (55%)	-1.64	0 100 100	29, 48, 68, 85	0
1	U	178/227 (78%)	-1.54	0 100 100	34, 52, 93, 109	0
1	Y	121/227 (53%)	-1.46	0 100 100	34, 56, 77, 89	0
1	c	98/227 (43%)	-1.07	0 100 100	83, 102, 112, 124	0
2	B	213/218 (97%)	-1.61	0 100 100	26, 49, 95, 103	1 (0%)
2	F	213/218 (97%)	-1.67	0 100 100	26, 47, 74, 95	1 (0%)
2	J	110/218 (50%)	-1.49	0 100 100	43, 58, 75, 83	0
2	N	213/218 (97%)	-1.66	0 100 100	26, 46, 73, 99	1 (0%)
2	R	110/218 (50%)	-1.46	0 100 100	45, 61, 84, 145	0
2	V	200/218 (91%)	-1.45	0 100 100	29, 58, 117, 131	0
2	Z	108/218 (49%)	-1.29	0 100 100	60, 82, 98, 107	0
2	d	81/218 (37%)	-1.08	0 100 100	81, 104, 116, 119	0
3	C	214/214 (100%)	-1.68	0 100 100	27, 48, 70, 105	0
3	G	214/214 (100%)	-1.66	0 100 100	29, 49, 70, 91	0
3	K	212/214 (99%)	-1.65	0 100 100	27, 49, 67, 79	0
3	O	214/214 (100%)	-1.61	0 100 100	29, 50, 81, 102	0
3	S	214/214 (100%)	-1.60	0 100 100	35, 57, 78, 110	0
3	W	200/214 (93%)	-1.42	0 100 100	36, 66, 98, 109	0
3	a	214/214 (100%)	-1.55	0 100 100	33, 61, 89, 110	0
3	e	214/214 (100%)	-1.46	0 100 100	49, 73, 92, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9	
4	D	220/226 (97%)	-1.64	0	100 100	27, 43, 87, 141	5 (2%)
4	H	219/226 (96%)	-1.65	0	100 100	26, 43, 88, 137	0
4	L	217/226 (96%)	-1.57	0	100 100	29, 47, 82, 180	1 (0%)
4	P	216/226 (95%)	-1.62	0	100 100	26, 43, 79, 141	2 (0%)
4	T	213/226 (94%)	-1.59	0	100 100	29, 43, 76, 174	1 (0%)
4	X	215/226 (95%)	-1.51	0	100 100	29, 51, 101, 187	0
4	b	217/226 (96%)	-1.57	0	100 100	30, 45, 77, 171	2 (0%)
4	f	215/226 (95%)	-1.41	0	100 100	46, 70, 104, 155	5 (2%)
All	All	5938/7080 (83%)	-1.56	0	100 100	24, 52, 97, 187	19 (0%)

There are no RSRZ outliers to report.

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PCA	b	1	8/9	0.96	0.10	20,20,20,20	0
4	PCA	L	1	8/9	0.97	0.06	20,20,20,20	0
2	PCA	V	1	8/9	0.97	0.12	20,20,20,20	0
2	PCA	N	1	8/9	0.98	0.09	20,20,20,20	0
4	PCA	P	1	8/9	0.98	0.06	20,20,20,20	0
4	PCA	T	1	8/9	0.98	0.05	20,20,20,20	0
2	PCA	F	1	8/9	0.98	0.07	20,20,20,20	0
4	PCA	X	1	8/9	0.99	0.04	20,20,20,20	0
4	PCA	H	1	8/9	0.99	0.05	20,20,20,20	0
4	PCA	D	1	8/9	1.00	0.04	20,20,20,20	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.